Synthesis and Characterization of Pr^{3+} doped CdS Nanomaterial

Jitendra Pal Singh[1*], Priyanka Goyal[1], Yogesh Kumar Sharma[2*], Raghavendra Prakash Dubedi[3]

Corresponding Author:[*]*drysharma@yahoo.com*

[1]*Department of Physics, Govt. P. G. College, Rudrapur (U S Nagar) Uttarakhand, India*

[2]*Deartment of Physics, Dr S.N. Govt. Post Graduate College, Karnprayag (Chamoli) Uttarakhand, India*

[3]*H.O.D. Chemistry, Govt. Degree College Churiyala, (Haridwar) Uttarakhand, India*

Abstract:

Cadmium sulfide (CdS) Nanoparticles doped with 0.1mol % praseodymium ion (Pr^{3+}) were synthesized by simple chemical precipitation method. The prepared CdS:Pr^{3+} nanomaterial have been characterized by powder X-ray diffraction studies (PXRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), EDAX, and FTIR at room temperature. Particle size (D) of nanomaterial and various parameters such as inter planar spacing (d), micro strain (ε), dislocation density (ρ) and distortion parameter (g) were computed. The CdS:Pr^{3+}nanomaterial exhibits spherical shape. The particle size is 4 nm to 37 nm estimated from PXRD.

Key words: CdS:Pr^{3+}nanomaterial, PXRD, SEM and FTIR

Introduction:

CdS nanoparticles are known for their extensive applications dual semiconducting and luminescence properties and show a great promise in medical imaging and treatment of disease. Nano size particles of semiconductor materials have gained much more interest in recent years due to their desirable properties and applications in different areas such as catalysts [1], sensors [2], photoelectron devices [3, 4], highly functional and effective devices [5]. CdS nanomaterial have novel electronic, structural, and thermal properties which are of high scientific interests in basic and applied fields [6]. CdS nano particles are also used as pigment in paints and in engineered plastic due to their good thermal stability [7]. CdS have large band gap energy of 2.42eV at room temperature that enables its nanoparticles to be remarkable in optoelectronics, photonics, photovoltaic can be used in optoelectronics for marking photocells, light emitting diode (LED) [8], and Lasers field effect transistor [9]. In photonics, due to its photo conducting and electrical properties can be used in sensors, photo detectors, optical filters, and optical switches, its band gap appears in the visible spectrum [10]. The useful for many commercial and potential application in photovoltaic, as hetero junction solar cells and thin film solar cells. In photo catalysis owing to its

photo chemicals and catalytic properties, Cds nanoparticles can be used for water splitting [11, 12] as well as for water and air purification.

Now a day's more emphasis has given to surface and interfaces roles in various research areas like nanotechnology and environmental technology etc. Template directed synthesis of nanoscale materials has found to have various potential applications in photo catalysis, molecular electronics, active electronic devices and solar energy conversion [13,14]. The utilization of template molecules in the nanomaterial fabrication increases the accessibility for catalytic reactions and are currently being explored in various systems like metal oxide, silica, aluminium hydroxide coated phospholipid tubules, cellulose, polymers, carbon nanotubes etc [13,14]. Among these materials biological templates are exploited more to modulate the synthesis of large number of inorganic nanoparticles including semiconductors, metals and magnetic particles. CdS similar to ZnS occurs in two crystalline forms with the hexagonal wurtzite as the most stable structure and the cubic zinc blende.

In present research paper, The Cadmium sulfide nanoparticles (CdS) doped with 0.1 mol % praseodymium (Pr^{3+})ion were synthesized by chemical precipitation synthesis method and characterized by PXRD, SEM, TEM, EDAX, and FTIR.

Experimental Details:

The CdS : Pr^{3+} nanomaterial were synthesized by simple chemical precipitation synthesis method [15]. All the chemicals were of analytical grade and were used without further purification. Cadmium nitrate tetrahydrate [$Cd(NO_3)_2.4H_2O$], sodium sulphide [Na_2S], diethylene glycol [DEG], ethanol [C_2H_5OH], praseodymium chloride [$PrCl_3$] and distilled water were used as a source material. 0.1M of $Cd(NO_3)_2.4H_2O$ (50ml) was taken in conical flask. Around 20 ml of diethylene glycol (DEG) was added to cadmium Nitrate tetrahydrate solution under constant stirring. After 15 minutes, 50 ml Sodium sulphide solution and (0.1 mol %) praseodymium chloride were added drop wise under constant stirring, reaction was kept 4hrs (at 60^0C) at constant stirring and yellow precipitate of CdS formed, washed with ethanol and distill water, dried at room temperature [15,16]. The flow chart of precipitation chemical synthesis method is shown in Fig.1. The prepared samples were characterized by PXRD, TEM, SEM, EDAX, and FTIR at room temperature. Characterization of CdS:Pr^{3+} nanomaterial have been done by courtesy of Indian Institute of Technology, Roorkee, India.

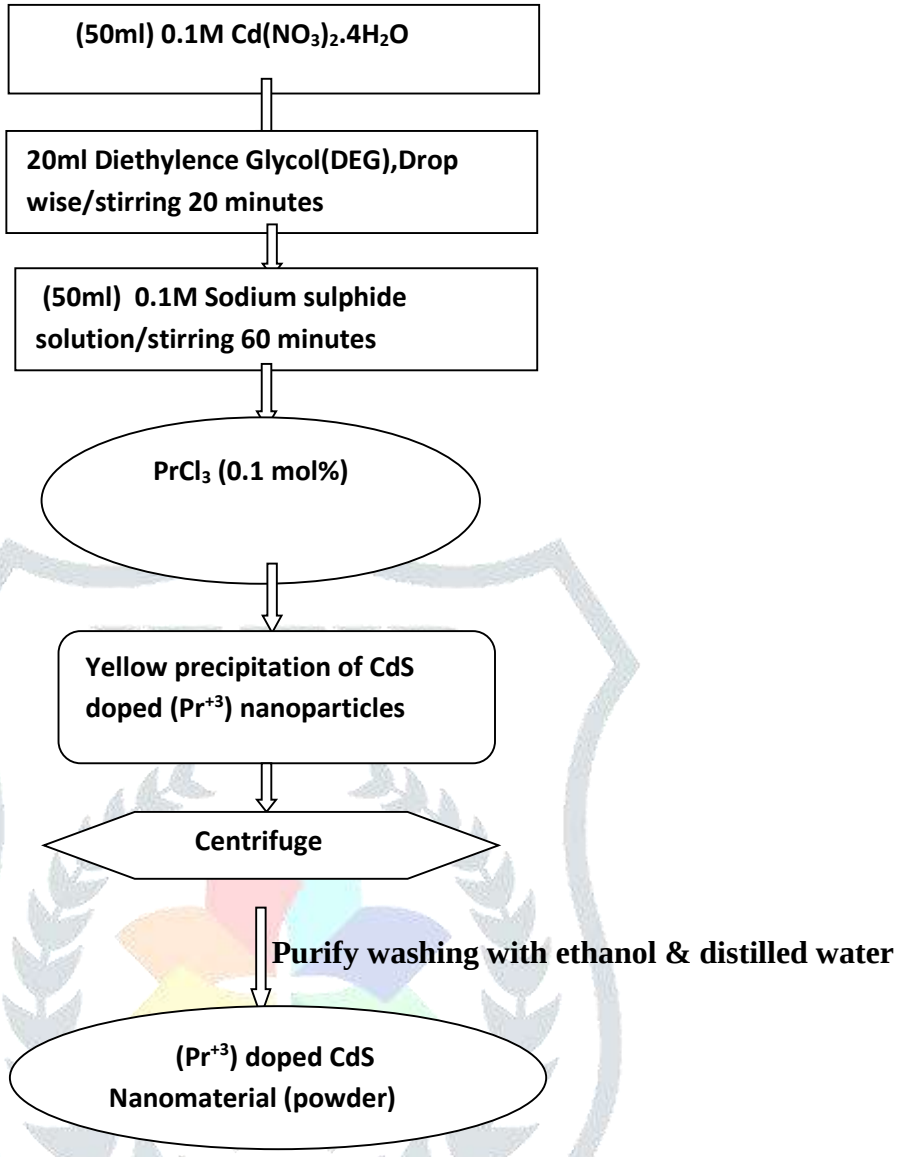

Fig 1: A flow chart Diagram of synthesis of CdS Nanomaterial with Pr^{+3}ions

Result and Discussion:

The CdS: Pr^{3+} nanomaterial have been synthesized by chemical precipitation synthesis method and characterized by PXRD, TEM, SEM, EDAX, and FTIR. Particle size and Physical various properties of nanomaterial have been computed.

PXRD patterns of nanoparticles were obtained using X-Pert Pro XRD spectrometer (P analytical B.V. Holland) from 10 to 80 degree (2Θ) value using Cu K-α radiation wavelength-0.15418nm. The PXRD spectrum of CdS:Pr^{3+} nanomaterial doped with 0.1 mol % Pr^{3+} ion is shown in Fig 2. The synthesized particles produce highly intense X- ray reflections in their corresponding PXRD pattern indicating that all the materials are crystalline in nature. Fig.2 is suggesting that incorporation of Pr^{3+} ion in the sample does not introduce appreciable changes in

the crystal structure of CdS. This shows that the hexagonal structure is not modified by the addition of Pr^{3+} ion into CdS materials. However, a small deviation in full width at half maxima of diffraction peaks was observed by the addition of doping ions, which may be due to a small variation in the size of Pr^{3+} ions. Particle size was determined from the width of XRD peaks using Scherrer's formula [17].

$$D= (0.94\ \lambda) / (\beta \cos \theta)$$

where β is the FWHM (Full Width at Half Maximum) of diffraction peaks, θ is the diffraction angle, λ is the wavelength of X rays and D is the crystalline size.

Various parameters such as interplanar spacing (d in Å), microstrain (ε), dislocation density (ρ in 10^{15} m/m^3) and distortion parameter (g) along the most intense peak were calculated using following well known equations and are shown in Table 1. The equations used are:

$$d = \lambda /2\sin \theta$$

$$\varepsilon = \beta \cos \theta/4$$

$$\rho = 1/D^2 \text{ and } g = \beta / \tan \theta$$

From Table 1, the particle size shows 3.38 – 37.8 nm. The variation in particle size occurs due to the interaction between the dopants and grain boundaries and this result in change in grain boundary energy. This leads to the stabilization of the surfaces/grain boundaries and variation in particle size. Also, it is clear from above equations that microstrain values decrease with increase in the crystallite size[18].

TEM images of the CdS nanoparticles are shown in Fig 3. Nearly Spherical shapes for the dark spots in the images indicate that the CdS nanoparticles are almost spherical. The estimated average particles size is 200nm.

The surface morphological of synthesized CdS: Pr^{3+} nanomaterial examined by SEM with different magnification level at room temperature. The SEM images of the CdS: Pr^{3+} nanomaterial were shown in Fig 4. The image shows that approximate more spherical shape with some tiny alterations and size of the particles around 1μ-200nm, which is in high correlation with XRD data. It demonstrates clearly the formation of spherial CdS nanoparticles and slightly change of morphology of the nanoparticles with the Pr^{3+} ions.

The EDAX spectrum of CdS: Pr^{3+} nanomaterial doped with 0.1 mol % praseodymium ion is shown in fig 5. These spectra reveal that all the elements are present in the final composition which is take initially.

Infrared spectrum is formed as a consequence of the absorption of the absorption of the electromagnetic radiation at frequency that vibration of specific sets of chemical bonds within a molecules.The experimental informed pattern is show in range of 4000cm^{-1}, show in fig 6. The

FTIR spectra is very much useful for structural analysis. The present of hydrogen and Oxygen is the useful characteristic CdS doped Pr^{3+}(0.1 mol %) in all infrared group. The absorption peak in the range of 3201-3326 could be attributed to the –OH group of water absorbed by samples. The peak around 1622-1644 cm^{-1} is assigned to the asymmetric stretching vibration of Cd-S bond from sulfur group. The peak in range 540-612 cm^{-1} are due to Pr^{3+} bond doped CdS nanoparticles.

Conclusions

The CdS nanoparticles doped with 0.1 mol% of Pr^{3+} ion means a nanomaterial have been prepared by a simple cost effective and eco-friendly precipitation chemical synthesis method. Structural and morphological composition were studied after a successfully synthesis and characterized by using different techniques such PXRD, SEM, TEM, FTIR and EDAX. The XRD study revealed the spherical wurtzite structure without second phase. The TEM images confirmed the spherical morphology of the nano material with size in the quantum dots range.

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Table 1: Various parameters computed from PXRD data for CdS:Pr^{3+} nanomaterial doped with 0.1 mol % Pr^{3+} ion

Peak position 2-theta(in deg)	**Particle size D (in nm)**	**FWHM β (in deg)**	**d-value (Å) observed**	**Dislocation density ρ (in 10^{15} m/m^3)**	**Distortion Parameter g**
15.72	**21.72**	**0.37**	**5.63**	**0.21**	**0.046**
28.49	**29.36**	**0.28**	**3.13**	**0.11**	**0.019**
33.06	**37.15**	**0.22**	**2.70**	**0.072**	**0.013**
36.47	**17.11**	**0.49**	**2.46**	**0.34**	**0.025**
38.74	**20.55**	**0.41**	**2.32**	**0.23**	**0.020**
56.40	**29.42**	**0.30**	**1.64**	**0.11**	**0.010**
59.19	**17.90**	**0.51**	**1.56**	**0.31**	**0.015**
70.72	**3.38**	**2.88**	**1.33**	**9.0**	**0.070**
76.93	**24.35**	**0.41**	**1.23**	**0.16**	**0.009**

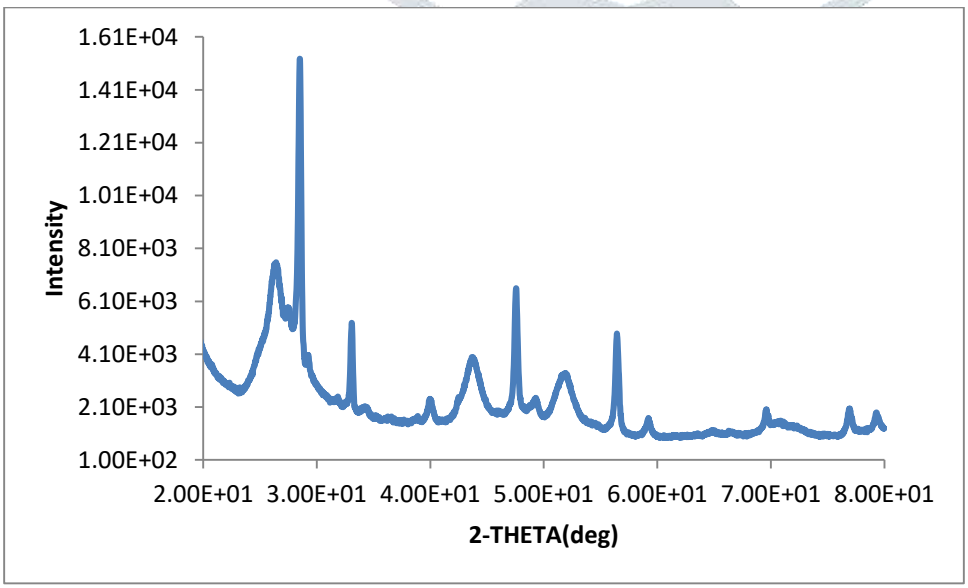

Fig 2: PXRD spectrum of CdS: Pr^{3+} nanomaterial doped with 0.1% mol Pr^{3+} ion

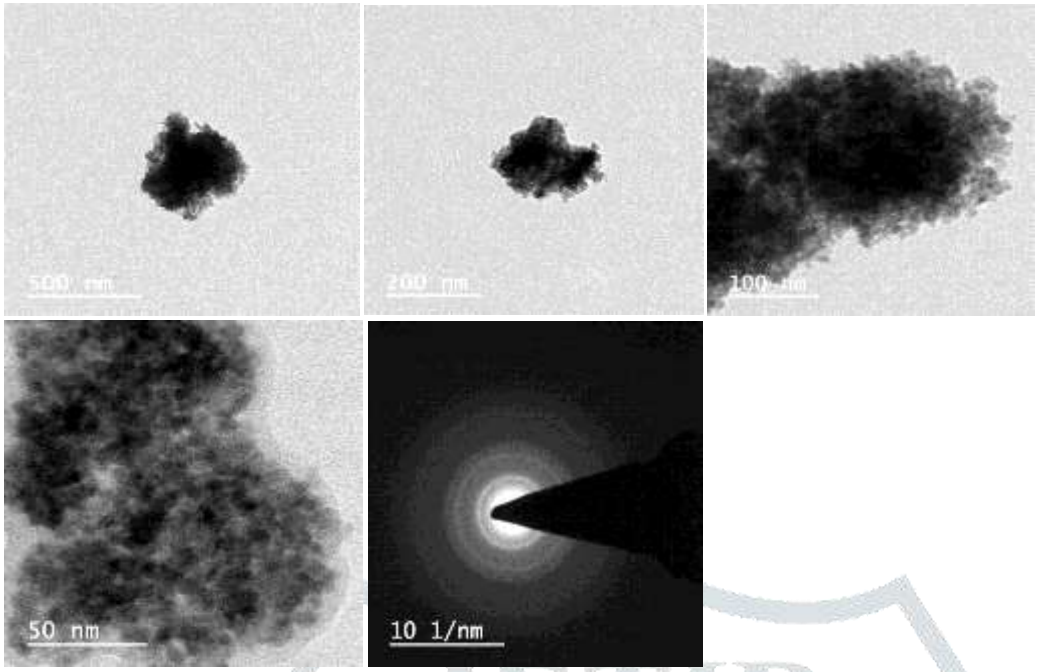

Fig 3. : TEM micrograph of CdS: Pr^{3+} nanomaterial doped with 0.1mol% Pr^{3+}ion

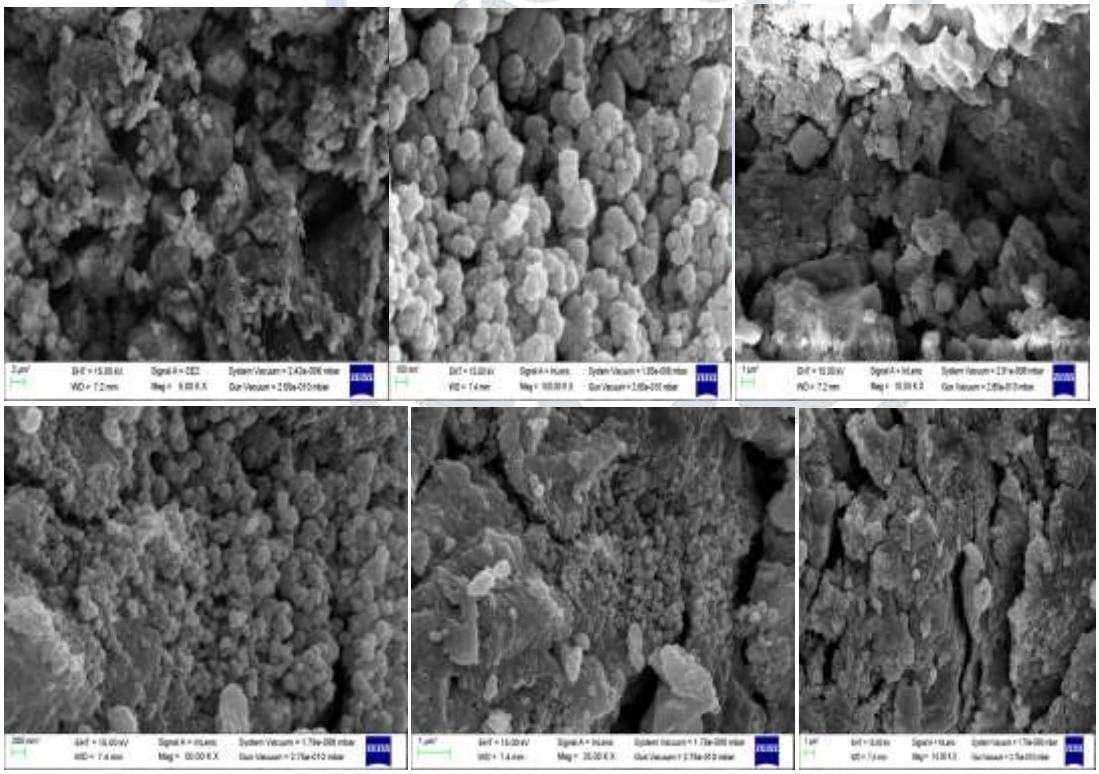

Fig 4 –SEM micrograph of CdS: Pr^{3+} nanomaterial doped with 0.1% Pr^{3+}ion.

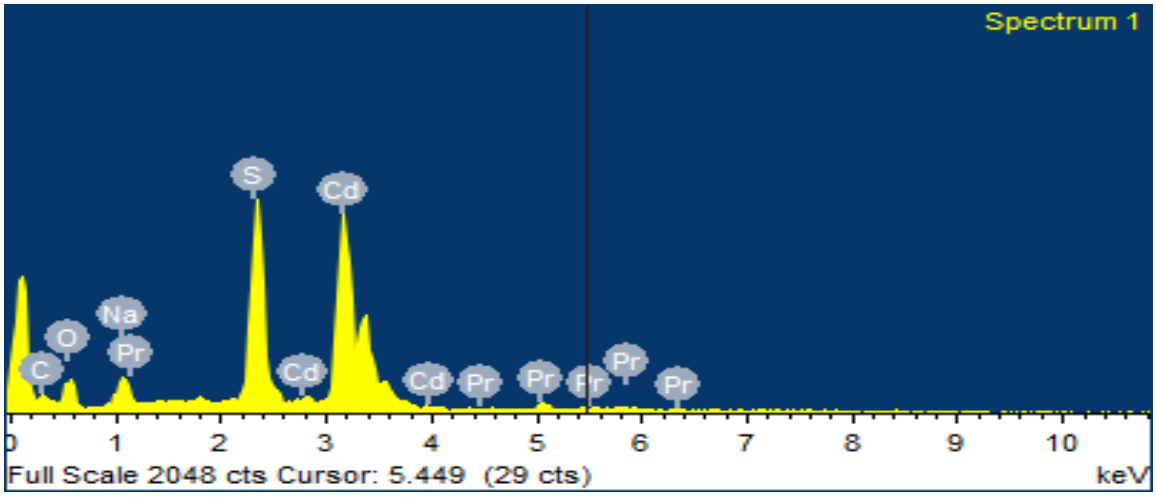

Fig 5 : EDAX spectrum of CdS: Pr^{3+} nanomaterial doped with 0.1mol% Pr^{3+}ion.

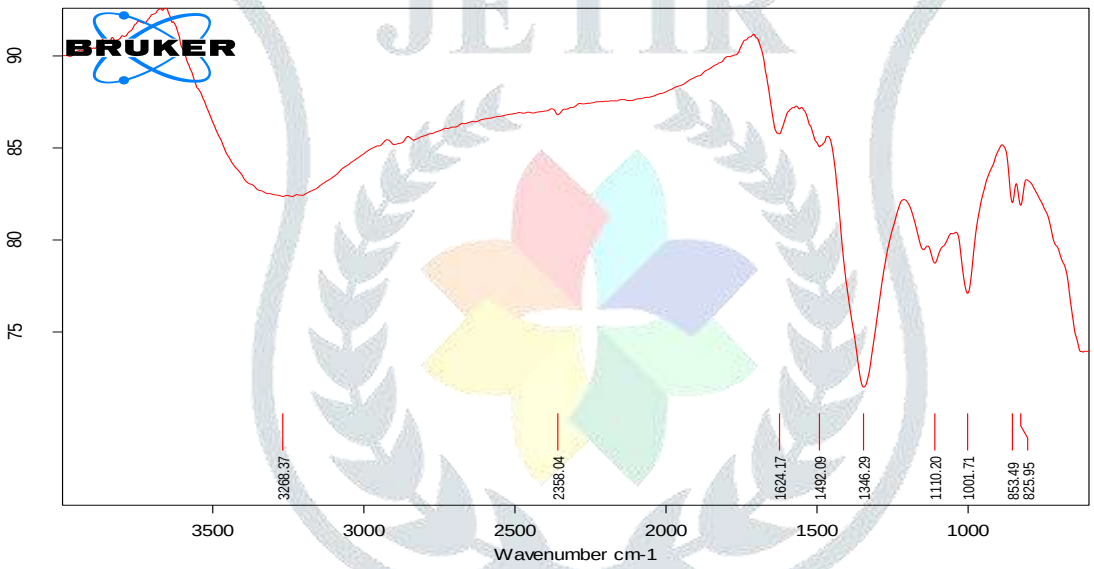

Fig 6. : FTIR spectrum of CdS: Pr^{3+} nanomaterial doped with 0.1mol%Pr^{3+} ion.